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FINITE ELEMENT ANALYSIS OF DAMAGE-HEALRING BEHAVIOUR IN SELF-HEALING CERAMIC MATERIALS

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Abstract. In this study, we develop the constitutive model to analyse the self-healing ceramic materials within the framework of FEM. The self-hearing and isotropic damage constitutive model for ceramic materials can describe not only the damage process under a certain boundary condition, but also the self-healing process under a high-temperature condition. The damage process is formulated based on the fracture mechanics, and the self-healing process is formulated based on the kinetic model of self-healing time and velocity. Then, we apply the proposed model to analyses of homogeneous ceramic materials and unit cell model of fiber-reinforced ceramic material.

1 INTRODUCTION

The self-healing fiber-reinforced ceramic material (shFRC) developed by the authors is a new functional material [1-3]. The self-crack/damage-hearing function is one of most valuable phenomena to overcome the reliability decrease of blittle ceramics that are caused by non-acceptable cracking. When a micro-crack propagates in this material, the self-healing occurs under high-temperature. Then, the strength of the material recovers to its initial state because the crack is re-bonded. The reason why the self-crack/hearing automatically attains the complete recovery of damaged strength is that the passive oxidation of self-healing agent, for example SIC, is caused by a crack itself. However, in order to apply the self-hearing ceramic material to machines and constractions, it is important to develop the novel numerical simulation method.

In this study, we develop the constitutive model to analyse the self-healing ceramic materials within the framework of FEM. The damage process is formulated based on the fracture mechanics [3], and the self-healing process is formulated based on the kinetics of self-healing time and velocity [1]. Therefore, the proposed self-hearing and isotropic damage constitutive model for ceramic materials can describe not only the damage process under a certain boundary condition, but also the self-healing process under a high-temperature condition. Then, we apply the proposed model to FE analyses of homogeneous ceramic material and unit cell model of ceramic matrix composites.

2 CONSTITUTIVE EQUATION

To formulate both the isotropic damage and self-healing behavior, we adopt the damage constitutive equation proposed by Kurumatani et al.[4]. In this model, the strain softening behavior due to damage is formulated based on the fracture mechanics of concrete material. Concretely, the critical energy release rate and the work due to the cohesive force and relative displacement relation are related, i.e. the damage behavior is described like a cohesive element model. In addition, the dependence on mesh size and mesh kind can be reduced because the size of finite element is incorporated as a characteristic length. In the following, first, we will explain the formulation under one-dimensional problem. Then, we will explain about the extension to three-dimensional problem using equivalent strain. Finally, we will explain about the evolution rule for self-healing behavior based on kinetics.

2.1 Formulation for one-dimensional problem

The one-dimensional damage model is described using scalar variable D as follows:

$$\sigma = (1-D)E\varepsilon \tag{1}$$

where σ, ε and E are stress, strain and Young's modulus, respectively. The damage variable D $(0 \le D \le 1)$ prescribes magnitude of damage, i.e. D=0 is a non-damage state and D=1 is a perfectly fracture state.

We assume that the relation of cohesive force and relative displacement (crack opening displacement) is expressed by an exponential function. Thus, the relation of cohesive force and crack opening displacement by tensile fracture in one-dimensional problem is given by the following equation.

$$f = Ae^{-Bw} \tag{2}$$

where f is the cohesive force on fracture surface, w is the crack opening displacement. And A and B are unknown parameters. If we assume f_t is one-dimensional tensile fracture strength, we can obtain the unknown parameter A as follows:

$$f_t = Ae^0 \rightarrow A = f_t \tag{3}$$

The fracture energy G_f is given as

$$G_f = \int_0^\infty f dw = A\int_0^\infty e^{-Bw} dw \tag{4}$$

Thus, the unknown parameter B is obtained as follows:

$$G_f = \frac{A}{B} \to B = \frac{A}{G_f} = \frac{f_t}{G_f} \tag{5}$$

Consequently, the relation of cohesive force and crack opening displacement in one-dimensional problem is obtained as follows:

$$f = f_t \exp\left(-\frac{f_t}{G_f} w \right) \tag{6}$$

In the following, Eq.(6) based on the fracture energy is applied to the damage constitutive model. An strain corresponding to the tensile strength is defined as the initial damage strain ε_0 and is given by

$$\varepsilon_0 = \frac{f_t}{E} \tag{7}$$

The crack opening displacement w is given by the relationship between displacement and strain as follows:

$$w = \varepsilon h_e - \varepsilon_0 h_e = (\varepsilon - \varepsilon_0) h_e \tag{8}$$

where h_e stands the length of finite element. In the damage model, the cohesive force (traction) f on the fracture surface is equivalent to stress σ, as the following equation.

$$f = \sigma \tag{9}$$

The relation of cohesive force and crack opening is obtained from Eqs. (6)-(9), as follows:

$$\begin{aligned}\sigma &= E\varepsilon_0 \exp\left(-\frac{E\varepsilon_0 h_e}{G_f}(\varepsilon - \varepsilon_0) \right) = \left[1 - \left\{ 1 - \frac{\varepsilon_0}{\varepsilon} \exp\left(-\frac{E\varepsilon_0 h_e}{G_f}(\varepsilon - \varepsilon_0) \right) \right\} \right] E\varepsilon \\ &= [1 - D(\varepsilon)] E\varepsilon\end{aligned} \tag{10}$$

Representing ε in the damage variable $D(\varepsilon)$ by the maximum strain $\bar{\varepsilon} \geq 0$ during deformation history, the damage variable $D(\bar{\varepsilon})$ is rewritten as follows:

$$D(\bar{\varepsilon}) = 1 - \frac{\varepsilon_0}{\bar{\varepsilon}} \exp\left(-\frac{E\varepsilon_0 h_e}{G_f}(\bar{\varepsilon} - \varepsilon_0) \right) \tag{11}$$

We can judge the loading criterion in accordance with the magnitude relationship between ε and $\bar{\varepsilon}$, i.e.

$$\begin{cases} \text{if } \ \bar{\varepsilon} \leq \varepsilon \to \bar{\varepsilon} = \varepsilon \text{ (loading)} \\ \text{if } \ \bar{\varepsilon} > \varepsilon \to \bar{\varepsilon} = \bar{\varepsilon} \text{ (unloading)} \end{cases} \tag{12}$$

In addition, the judgment of damage is given as follows:

$$\begin{cases} \text{if } \ \varepsilon < \varepsilon_0 \to D = 0 \text{ (undamage)} \\ \text{if } \ \varepsilon \geq \varepsilon_0 \to D = D(\bar{\varepsilon}) \end{cases} \tag{13}$$

2 Formulation for three-dimensional problem

In general, the equivalent strain, which is scalar value, is used for the isotropic damage model in multi-dimensional problems. Kurumatani et al.[4] have adopted the following equivalent strain ε_{eq} based modified von-Mises type [5].

$$\varepsilon_{eq} = \frac{k-1}{2k(1-2\nu)} I_1 + \frac{1}{2k}\sqrt{\left(\frac{k-1}{1-2\nu} I_1\right)^2 + \frac{12k}{(1+\nu)^2} J_2} \tag{14}$$

where ν is Poisson's ratio, and k is a ratio of the compressive and tensile strengths. I_1 is the first invariant of strain tensor $\boldsymbol{\varepsilon}$ and is given by

$$I_1 = \mathrm{tr}\boldsymbol{\varepsilon} = \varepsilon_{kk} \tag{15}$$

J_2 is the second invariant of deviatoric strain tensor $\boldsymbol{\varepsilon}^*$ and is given by

$$J_2 = \frac{1}{2}\boldsymbol{\varepsilon}^* : \boldsymbol{\varepsilon}^* = \frac{1}{2}\varepsilon^*_{kl}\varepsilon^*_{kl} \tag{16}$$

The deviatoric strain is defined by

$$\boldsymbol{\varepsilon}^* = \boldsymbol{\varepsilon} - \frac{1}{3}\mathrm{tr}\boldsymbol{\varepsilon}\mathbf{I} \tag{17}$$

Here, $\mathbf{I}$ is unit tensor.

Next, we will describe the stress-strain relation in multi-dimensional problem. The isotropic damage model is described using damage variable D as follows:

$$\boldsymbol{\sigma} = (1-D)\mathbf{c} : \boldsymbol{\varepsilon} \tag{18}$$

where $\boldsymbol{\sigma}$ is Cauchy stress tensor, $\mathbf{c}$ is elastic coefficient tensor. In this study, we adopt the hypo-elastic coefficient tensor.

By using the maximum value of equivalent strain $\kappa \geq 0$ in deformation history, the damage variable $D(\kappa)$ is given as follows:

$$D(\kappa) = 1 - \frac{\kappa_0}{\kappa}\exp\left(-\frac{E\kappa_0 h_e}{G_f}(\kappa - \kappa_0)\right) = 1 - \frac{\kappa_0}{\kappa} e^{-\beta(\kappa-\kappa_0)} \tag{19}$$

where κ_0 is the initial damage strain. In what follows, κ is called the history variable or the maximum equivalent strain. The length of three-dimensional solid element is defined based on the volume V_e as follows:

$$h_e = V_e^{1/3} \tag{20}$$

The loading criterion is given by

$$\begin{cases} \text{if } \ \kappa \leq \varepsilon_{eq} \to \kappa = \varepsilon_{eq} \text{ (loading)} \\ \text{if } \ \kappa > \varepsilon_{eq} \to \kappa = \kappa \text{ (unloading)} \end{cases} \tag{21}$$

$$\begin{cases} \text{if } \ \kappa < \kappa_0 \to D = 0 \text{ (undamage)} \\ \text{if } \ \kappa \geq \kappa_0 \to D = D(\kappa) \end{cases} \tag{22}$$

2.3 Evolution rule for self-hearing

To incorporate the self-healing behavior to the damage constitutive model, we assume that a micro cracks (damage) are recovered by self-healing function. In other words, the damage variable is varied from the damage state $D \neq 0$ to the non-damage state $D = 0$ in accordance with the self-healing that is affected by the temperature and atmosphere conditions. Thus, we assume that the history variable κ evolves to be closer to κ_0 with the self-healing. That is, the damage history is gradually dissipated by the self-healing. Based on abobe-mentioned concept, we will formulate the evolution rule for self-healing.

First, we assumed that the history variable is additively decomposed into the equivalent strain part κ_ε and the self-healing part $-\kappa_h$ as follows:

$$\kappa = \kappa_\varepsilon - \kappa_h \tag{23}$$

where the contributed part by progress of equivalent strain ε_{eq} is given as

$$\kappa_\varepsilon = \int_t \dot{\varepsilon}_{eq} dt \quad \text{if} \quad \varepsilon_{eq} \geq \bar{\kappa} \tag{24}$$

$$\kappa_\varepsilon = \kappa_\varepsilon + < \Delta\varepsilon_{eq} > \tag{25}$$

On the other hand, the self-healing part κ_h is assumed a monotonic increasing function to approach the state $\kappa \to \kappa_0$. we then assume the following simple function for the evolution rule of κ_h.

$$\dot{\kappa}_h = \xi_1 v_h \left(\kappa - \kappa_0\right) = \xi_1 v_h \left(\kappa_\varepsilon - \kappa_h - \kappa_0\right) \tag{26}$$

$$\kappa_h = \int_t \dot{\kappa}_h dt \approx \kappa_h + \dot{\kappa}_h dt \tag{27}$$

where ξ_1 is the parameter that influences the rate of self-healing. v_h [s^{-1}] is the average velocity of self-healing based on kinetics. In this study, we adopt the following equation proposed by Osada et al.[1].

$$v_h = \frac{1}{t_h^{\min}} = A_h \cdot \exp\left(\frac{-Q_h}{RT_h}\right) a_{O_2}{}^{3n/2} \tag{28}$$

where A_h is the frequency factor, Q_h is the activation energy for self-healing, R is the gas constant, and T_h is the temperature. a_{O_2} and n are the activity of Oxygen and the reaction order of Oxygen, respectively. Thus, we can consider $h_e \dot{\kappa}_h$ as a filling velocity of mcro-crack.

Furthermore, to describe that a restart of damage depends on a degree of the self-healing, the maximum equivalent strain $\bar{\kappa}$ has to be re-defined. In the loading state, as well as the normal damage model, $\bar{\kappa}$ is given by the following manners.

$$\bar{\kappa} = \max\{\kappa_\varepsilon\} \geq \kappa_0 \quad \text{for loading with damage} \tag{29}$$

On the other hand, in the self-healing state, we assume that the maximum equivalent strain $\bar{\kappa}$ gradually approaches to κ_0. We then assume the evolution rule of the maximum equivalent strain as follows:

$$\dot{\bar{\kappa}} = -\xi_2 v_h \left(\bar{\kappa} - \kappa_0\right) \tag{30}$$

$$\bar{\kappa} = \int_t \dot{\bar{\kappa}} dt \approx \bar{\kappa} + \dot{\bar{\kappa}} dt \tag{31}$$

That is, in the reloading state, the damage does not occur until $\min(\varepsilon_{eq},\ \kappa) \geq \bar{\kappa}$. Here, ξ_2 is the parameter that influences the rate of self-healing. Although the initial damage strain in the reloading state is $\bar{\kappa}$, strain necessary to reach it is adjusted by the magnitude of ξ_1 and ξ_2. In the case of $\xi_1 \geq \xi_2$, the super healing phenomenon, in which the fracture strength of healed material becomes higher than that of virgin material, is naturally described. Note that if we set the average velocity of self-healing to zero, i.e. $v_h = 0$, the condition $\kappa = \kappa_\varepsilon = \bar{\kappa}$ is satisfied, and thus the model becomes the normal damage model as described in Section 2.2.

By considering of the evolution rules for above-mentioned history variables, the loading criterion is summarized as follows:

$$\begin{cases} \text{if } \left\langle \Delta\varepsilon_{eq} \right\rangle > 0 \rightarrow \kappa_\varepsilon = \kappa_\varepsilon + \Delta\varepsilon_{eq} \text{ (loading)} \\ \text{if } \left\langle \Delta\varepsilon_{eq} \right\rangle = 0 \rightarrow \kappa_\varepsilon = \kappa_\varepsilon \text{ (unloading)} \end{cases} \tag{32}$$

$$\begin{cases} \text{if } \min(\varepsilon_{eq},\ \kappa) < \bar{\kappa} \rightarrow D = 0 \quad \text{for } \kappa < \kappa_0 \\ \text{if } \min(\varepsilon_{eq},\ \kappa) < \bar{\kappa} \rightarrow D = D(\kappa) \quad \text{for } \kappa \geq \kappa_0 \\ \text{if } \min(\varepsilon_{eq},\ \kappa) \geq \bar{\kappa} \rightarrow D = D(\kappa) \quad \text{for } \bar{\kappa} = \kappa \end{cases} \tag{33}$$

It should be noted that the following equations based on the logistic curve would be suitable for the evolution rule of self-healing, instead of Eqs.(26) and (30).

$$\dot{\kappa}_h = \xi_1 v_H \kappa_h (\kappa_\varepsilon - \kappa_0 - \kappa_h) \tag{34}$$

$$\dot{\bar{\kappa}} = -\xi_2 v_h \bar{\kappa} \left(\kappa_0 - \bar{\kappa}\right) \tag{35}$$

3 FINITE ELEMENT ANALYSIS

In this section, we demonstrate the analysis of damage and healing phenomena within the framework of continuum theory using the FEM implemented with the proposed model.

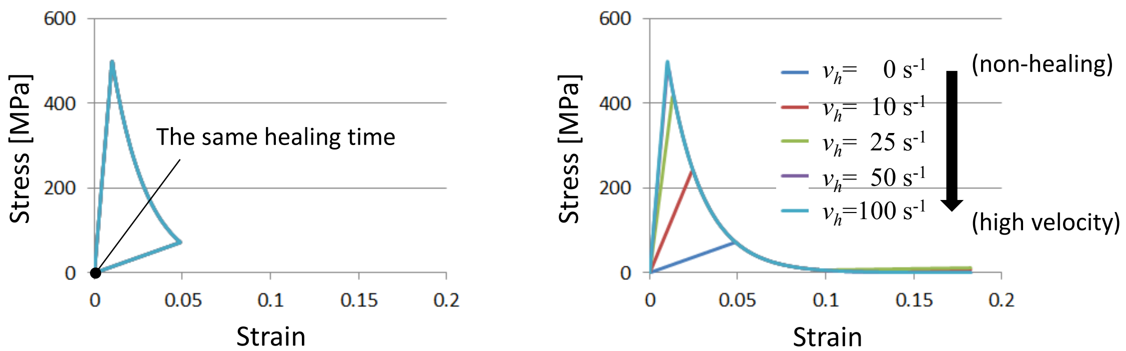
Table 1: Material parameters.

E [MPa]	50000	k	10
G [MPa]	25000	h_e [mm]	10
ν	0.3	v_h [s^{-1}]	0-100
G_f [J]	100	ξ_1	1.0
κ_0	0.01	ξ_2	1.0

3.1 Mechanical response of proposed model

In this study, the self-healing and isotropic damage model is implemented in the commercial FEM software package LS-DYNA Ver.971 [6]. To demonstrate the capability of the proposed model, we created a simplest FE model. The model is discretized by one eight-node solid element. The element is $10\times10\times10$ mm in size. Prescribed forced cycle displacement into uniaxial direction is imposed at upper surface. Material parameters used for the analysis is listed in Table 1. Note that, to reasonably verify the mechanical response of proposed model, we adopt quite high values for the average velocity of self-healing, v_h.

Figure 1(a) and 1(b) show the effect of v_h on the stress-strain relation under cyclic loading. Figure 1(a) and 1(b) present result of “loading-unloading-rest” and “reloading” states, respectively, where the healing time is the same for each condition. It can be confirmed from Figure 1 that the self-healing occurs during stop of loading and the fracture strength recovers in accordance with the average velocity of self-healing. Figure 2 shows the variation of damage variable D during cyclic loading as shown in Figure 1. By introducing of the evolution rule of Eqs.(26) and (30), the damage variable gradually approaches to zero. It is also confirmed that the variation rate of damage variable depends on v_h.



(a) Loading-unloading- rest

(b) Reloading

Figure 1: Effect of v_h on stress-strain relation under cyclic loading.

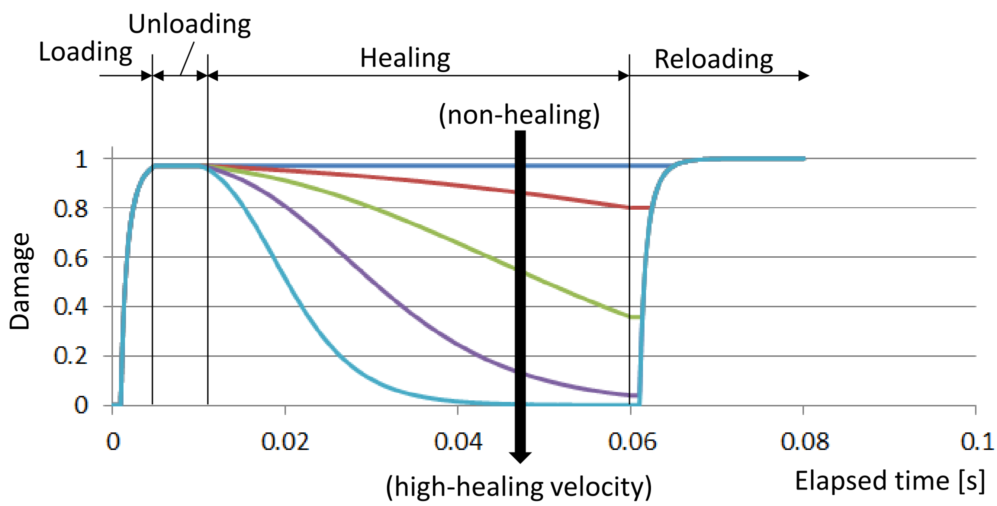
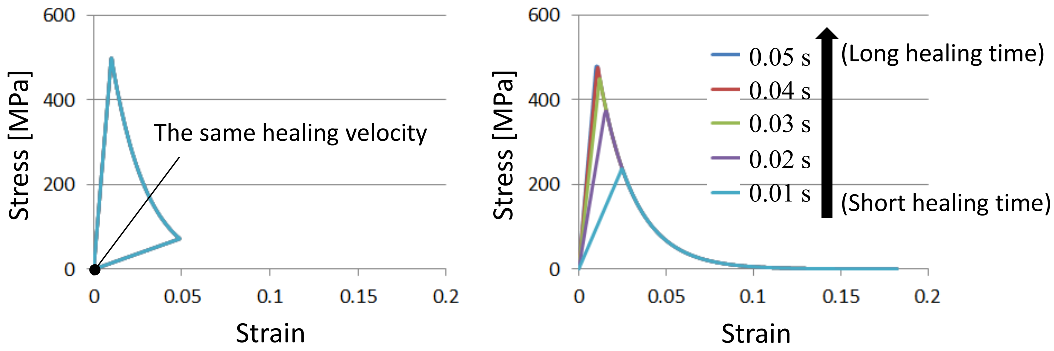


Figure 2: Variation of damage variable D during loading-rest-reloading.

Figure 3(a) and 3(b) show the effect of healing time on stress-strain relation under cyclic loading. Figure 3(a) and 3(b) present result of "loading-unloading-rest" and "reloading" states, respectively, where the average velocity of self-healing is the same for each condition. It can be confirmed from Figure 3 that the fracture strength recovers in accordance with the healing time.



(a) Loading-unloading- rest (b) Reloading

Figure 3: Effect of healing time on stress-strain relation under cyclic loading.

3.2 Analysis of unit cell model of fiber reinforced ceramic

Next, we analyze the damage and self-healing processes of ceramic matrix composite. Figure 4 shows the FE analysis model and imposed boundary conditions, where eight-node solid elements are adopted for discretization of ceramic matrix composite. In this study, we adopt the unit cell model of fiber reinforced ceramic matrix composite [2] for the analysis model. In the calculation, we apply the prescribed forced cyclic displacement to the side surface of unit cell. To reproduce the damage progress from matrix part, the initial defect is given as shown in Figure 4. Material parameters used for the analysis is listed in Table 2, while the fiber is assumed to an elastic material having $E = 80\,[\text{GPa}]$ and $\nu = 0.2$. Note that, to reasonably verify the mechanical response of proposed model, we adopt quite high values for the average velocity of self-healing, v_h.

Figure 5(a) and 5(b) show the relationship between nominal stress and nominal strain of unit cell under cyclic loading. Figure 5(a) and 5(b) present result of "normal damage model" and "self-healing and damage model", respectively, where the healing time is the same for each condition. Figure 6 shows the contour map of damage variable D during cyclic loading in the case of high healing velocity condition. As can be seen from Figures, the damaged region progresses from initial defect point and the stiffness of unit cell decreases during loading. After unloading, the self-healing occurs and the damaged region recovers to initial state as shown in Figure 6. Then, the fracture strength and stiffness are recovered according to the healing velocity v_h and the healing time. These results suggest that the proposed model can be applied to analyses of ceramic matrix composites having self-healing functions.

Table 2: Material parameters for fiber reinforced cermic.

E [MPa]	43200	k	10
G [MPa]	18000	h_e [mm]	0.008
ν	0.2	v_h [s^{-1}]	200, 2000
G_f [Nmm]	10	ξ_1	1.0
κ_0	0.0056	ξ_2	1.0

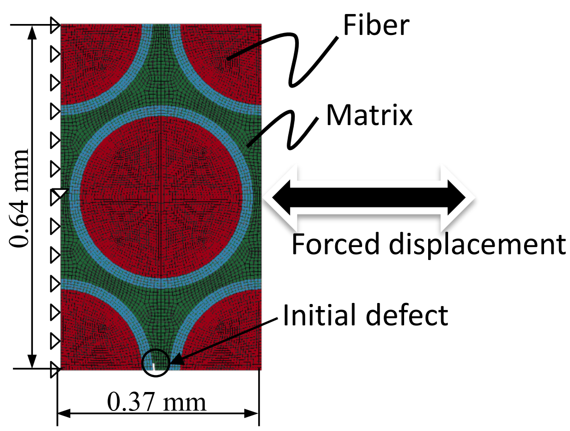
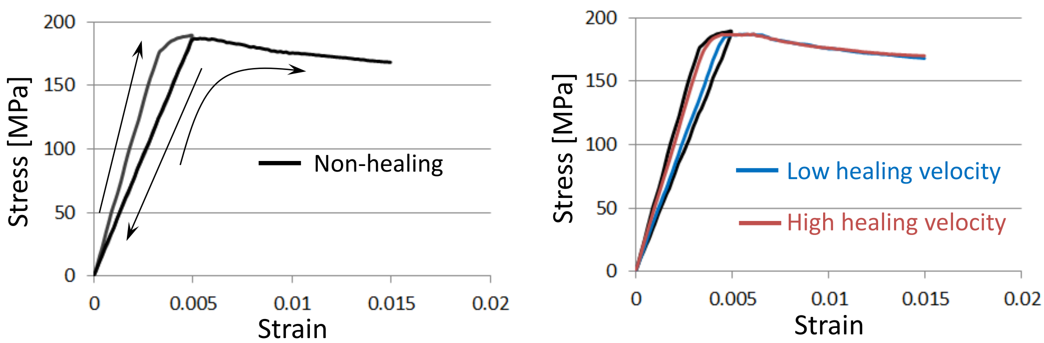


Figure 4: FE analysis model and boundary conditions of unit cell (thickness is 0.005 mm)



(a) Normal damage model (b) Self-healing and damage model

Figure 5: Relationship stress and strain of unit cell under cyclic loading.

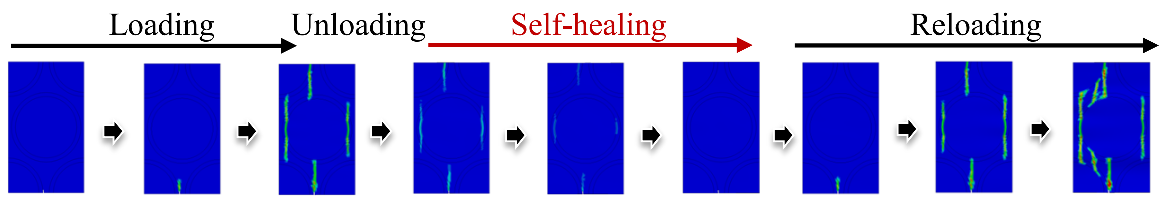


Figure 6: Contour map of damage variable during cyclic loading in the case of high healing velocity condition.

4 CONCLUSIONS

The present study formulated the self-healing and damage constitutive equation. We then applied it to the typical FE problems and then verified the formulation. The proposed model can describe the competition between the progress of damage and the self-healing by the unified formulation. Thus, the proposed model can be applied arbitrary deformation histories, including cyclic loading and strain holding. From the results of FE analyses, we can conclude that the present FE approach can be used to study the mechanical and material design of self-healing ceramic materials.

In the present FE analysis, however, the quite large values for healing velocity were adopted. Therefore, effects of temperature and oxygen conditions on healing velocity were not examined. Eq.(28) based on kinetics should be applied to FE analyses, in near future. Then, the verification of the concreate functions for the evolution rules should be performed by comparing with experiments.

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REFERENCES

[1] Osada, T., Nakao, W., Takahashi, K. and Ando, K. Kinetics of self-crack-healing of alumina/silicon carbide composite including oxygen partial pressure effect. *Journal of the American Ceramic Society* (2009) **92**:864-869.

[2] Nakao, W. and Haga, Y. *Dvelopment of selfhealing fiber reinforced ceramics matrix composite*, Japan Patent Kokai (2010) 2010-290947.

[3] Osada, T., Nakao, W., Takahashi, K. and Ando, K. Self-crack-healing behavior in ceramics matrix composite, *Advances in ceramics matrix composites* (2014) **17**: 410-441.

[4] Kurumatani, M., Terada, K., Kato, J., Kyoya, T. and Kashiyama, K. An isotropic damage model based on fracture mechanics for concrete and its evaluation, *Transactions of JSCES* (2013) No.20130015, *in Japanese*.

[5] de Vree, J.H.P., Brekelmans, W.A.M. and van Gils, M.A.J. Comparison of nonlocal approaches in continuum damage mechanics, *Comput. Struct.* (1995) **55**:581-588.

[6] LS-DYNA Ver.971, *Keywords manual & Theory manual*. LSTC (2012).